

# Quantum expectations via spectrograms

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We discuss a new phase space method for the computation of quantum expectation values in the high frequency regime. Instead of representing a wavefunction by its Wigner function, which typically attains negative values, we define a new phase space density by adding a first-order Hermite spectrogram term as a correction to the Husimi function. The new phase space density yields accurate approximations of the quantum expectation values as well as allows numerical sampling from non-negative densities. We illustrate the new method by numerical experiments in up to 128 dimensions.

## I. INTRODUCTION

Wigner functions are phase space functions that represent quantum states [1]. Among their important properties is the exact correspondence for expectation values via phase space integration. However, Wigner functions in general attain negative values. This phenomenon of “negative probabilities” also poses numerical problems when discretizing the phase space integrals by Monte-Carlo methods.

Spectrograms are a large class of non-negative phase space functions that result from coarse-graining the Wigner function by convolution with another Wigner function [2]. The most prominent spectrogram is the Husimi function [3], which is obtained by convolving with the Wigner function of a Gaussian. The drawback of the coarse-graining is the loss of the exact correspondence for expectation values.

Following the ideas of [4], we add first order Hermite spectrograms to the Husimi function. The resulting new phase space density is a linear combination of probability densities that approximates the Wigner function more accurately than the Husimi function, particularly

in calculating the expectation values of observables.

We proceed as follows. After a brief review of the relationship between expectation values and Wigner and Husimi functions as well as of spectrograms in §II, we construct the new density in §III and present supporting numerical experiments in §IV.

## II. QUANTUM EXPECTATIONS

### A. High frequency wavefunctions

Our goal is to compute quantum expectation values of observables  $\hat{A}$ ,

$$\langle \psi | \hat{A} | \psi \rangle =: \langle \hat{A} \rangle_\psi \quad (1)$$

for wavefunctions  $\psi : \mathbb{R}^d \rightarrow \mathbb{C}$  that are highly oscillatory with frequencies of the size  $O(h^{-1})$ , where

$$0 < h \ll 1$$

is a small parameter. In the context of the Born–Oppenheimer approximation,  $h$  is square root of the ratio of electronic versus average nuclear mass and typically ranges between  $10^{-3}$  and  $10^{-1}$ .

We assume that the observable  $\hat{A}$  arises as the Weyl quantization of its classical phase space

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counterpart  $A : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ ; see e.g. [5]. Then, expectation values can be computed via the integral formula

$$\langle \hat{A} \rangle_\psi = \int_{\mathbb{R}^{2d}} A(z) \mathcal{W}_\psi(z) dz, \quad (2)$$

where the Wigner function  $\mathcal{W}_\psi : \mathbb{R}^{2d} \rightarrow \mathbb{R}$  is the phase space symbol of the quantum state,

$$\widehat{\mathcal{W}}_\psi \propto |\psi\rangle\langle\psi|,$$

see e.g. [1, 5–7] or the monograph [8, §3].

### B. Phase space densities

Apart from Gaussian states, Wigner functions attain negative values and usually exhibit strong oscillations; see the illustration in Figure 1. Hence it is difficult to sample phase space points with respect to  $\mathcal{W}_\psi$  for the Monte Carlo quadrature of the integral (2). Our goal is to replace  $\mathcal{W}_\psi$  by a new phase space density with the following properties:

- the new density is built from smooth probability densities, so that (2) is amenable to positive sampling strategies;
- the new density approximates the Wigner function, so that (2) is exact for quadratic observables and holds approximately with a small error in general.

It is well-known that Husimi functions and spectrograms are analytic probability densities, but only provide exact expectation values for linear observables. However, an appropriate linear combination of Hermite spectrograms results in a phase space density that fulfills both our requirements.

### C. Spectrograms and Husimi functions

Non-negative phase space representations can be obtained by coarse-graining of the Wigner function. The spectrogram  $S_\psi^\phi : \mathbb{R}^{2d} \rightarrow [0, \infty)$

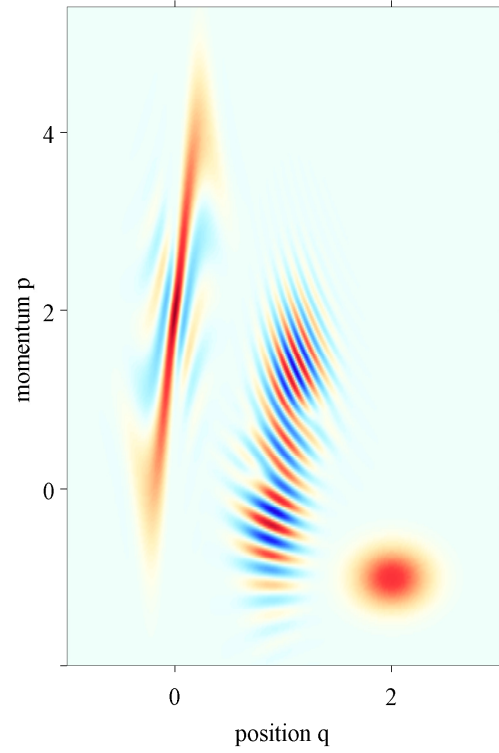


Figure 1. Contour plot of the Wigner function of a one-dimensional superposition of a Gaussian state (lower right) and a WKB type delocalized state (left). Blue coloring is used for negative values.

of a wavefunction  $\psi$  with respect to a smooth window function  $\phi : \mathbb{R}^d \rightarrow \mathbb{C}$  is defined as the convolution

$$\begin{aligned} S_\psi^\phi(z) &:= (\mathcal{W}_\psi * \mathcal{W}_\phi)(z) \\ &= \int_{\mathbb{R}^{2d}} \mathcal{W}_\psi(w) \mathcal{W}_\phi(z - w) dw. \end{aligned}$$

Whenever  $\psi$  and  $\phi$  are  $L^2$ -normalized,  $S_\psi^\phi$  is a smooth probability density on the phase space. Spectrograms are widely used in time-frequency analysis; see e.g. the introduction of [2].

The most popular spectrogram is the Husimi function,

$$\mathcal{H}_\psi := S_\psi^{g_0} = \mathcal{W}_\psi * \mathcal{W}_{g_0}, \quad (3)$$

see e.g. [3, 9], where the window is a Gaussian function

$$g_0(x) := (\pi h)^{-d/4} \exp(-\frac{1}{2h}|x|^2).$$

Replacing the Wigner function by the Husimi function in equation (2), we obtain

$$\langle \hat{A} \rangle_\psi = \int_{\mathbb{R}^{2d}} A(z) \mathcal{H}_\psi(z) dz + O(h), \quad (4)$$

where the error term vanishes for linear observables  $\hat{A}$ ; see also Figure 4.

### III. A NEW PHASE SPACE DENSITY

#### A. Combining Hermite spectrograms

We Taylor expand the Gaussian in the convolution defining the Husimi function

$$\mathcal{H}_\psi(z) = (\pi h)^{-d} \int_{\mathbb{R}^{2d}} \mathcal{W}_\psi(w) e^{-|z-w|^2/h} dw$$

around  $z$ , and obtain the asymptotic expansion

$$\mathcal{W}_\psi(z) = \mathcal{H}_\psi(z) - \frac{h}{4} \Delta \mathcal{H}_\psi(z) + O(h^2).$$

Substituting this expression into (2) yields

$$\langle \hat{A} \rangle_\psi = \int_{\mathbb{R}^{2d}} A(z) (1 - \frac{h}{4} \Delta) \mathcal{H}_\psi(z) dz + O(h^2),$$

where the error depends on fourth and higher order derivatives of  $A$ . We take a closer look at the Laplacian  $\Delta \mathcal{H}_\psi$ . Consider the rescaled first order Hermite functions

$$\varphi_j(x) = (\pi h)^{-d/4} \sqrt{\frac{2}{h}} x_j \exp(-\frac{1}{2h}|x|^2),$$

for  $j = 1, \dots, d$ . A direct calculation provides a first order Laguerre function in  $|z|^2/h$ ,

$$\mathcal{W}_{\varphi_j}(z) = -(\pi h)^{-d} (1 - \frac{2}{h}|z_j|^2) e^{-|z|^2/h}$$

for  $z = (z_1, \dots, z_d) \in \mathbb{R}^{2d}$ ; see also [10]. Thus,

$$\Delta \mathcal{W}_{g_0}(z) = \frac{2}{h} \sum_{j=1}^d \mathcal{W}_{\varphi_j}(z) - \frac{2d}{h} \mathcal{W}_{g_0}(z),$$

and then we conclude from (3) that

$$\Delta \mathcal{H}_\psi = \mathcal{W}_\psi * \Delta \mathcal{W}_{g_0} = \frac{2}{h} \sum_{j=1}^d S_\psi^{\varphi_j} - \frac{2d}{h} \mathcal{H}_\psi.$$

Now we define the new phase space density  $\mu_\psi : \mathbb{R}^{2d} \rightarrow \mathbb{R}$  by

$$\mu_\psi(z) := (1 + \frac{d}{2}) \mathcal{H}_\psi(z) - \frac{1}{2} \sum_{j=1}^d S_\psi^{\varphi_j}(z), \quad (5)$$

as a linear combination of the two smooth probability densities  $\mathcal{H}_\psi$  and  $\frac{1}{d} \sum_{j=1}^d S_\psi^{\varphi_j}$ ; see Figure 2 for an example. The new density satisfies

$$\int_{\mathbb{R}^{2d}} \mu_\psi(z) dz = \langle \psi | \psi \rangle^2$$

and provides quantum expectations as

$$\langle \hat{A} \rangle_\psi = \int_{\mathbb{R}^{2d}} A(z) \mu_\psi(z) dz + O(h^2). \quad (6)$$

The error term in (6) vanishes whenever  $A$  is a polynomial of degree less or equal to three. By including higher order Hermite spectrograms, one can derive similar densities that give exact expectation values for higher order polynomial observables; see [11].

#### B. Explicit formulas for $\mu_\psi$

One can find formulas for  $\mu_\psi$  when the state is a Gaussian wavepacket,  $\psi = g_z$ ,

$$g_z(x) := (\pi h)^{-d/4} \exp(\frac{i}{h} p \cdot (x - \frac{1}{2} q)) \times \exp(-\frac{1}{2h}|x - q|^2)$$

centered in  $z = (q, p) \in \mathbb{R}^{2d}$ , a Gaussian superposition,  $\psi = g_{z_1} + g_{z_2}$ , or a harmonic oscillator eigenstate,  $\psi = \varphi_k$ ,  $k \in \mathbb{N}^d$ ; see [4].

For instance, a Gaussian wave packet gives rise to the density

$$\mu_{g_z}(w) = (2\pi h)^{-d} \left(1 + \frac{d}{2} - \frac{|w-z|^2}{4h}\right) e^{-|w-z|^2/2h}.$$

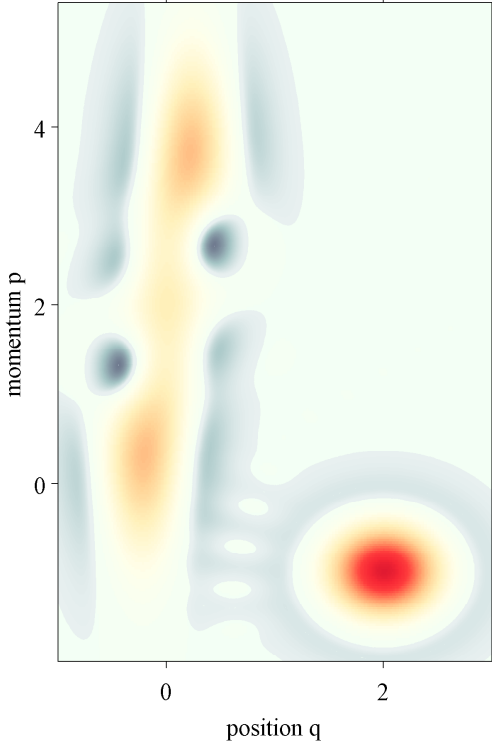


Figure 2. Contour plot of the density  $\mu_\psi$  for the same state as in Figure 1. Grey coloring is used to highlight regions of prominent negative values.

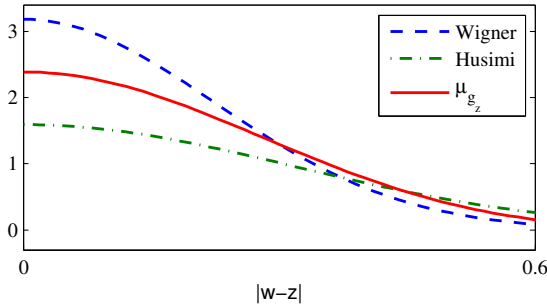


Figure 3. Section of the Wigner function  $\mathcal{W}_{g_z}(w)$ , the Husimi function  $\mathcal{H}_{g_z}(w)$ , and the density  $\mu_{g_z}(w)$  in dependence of  $|w - z|$ , where  $h = 10^{-1}$ .

Figure 3 illustrates that — due to the polyno-

mial prefactor — the density  $\mu_{g_z}$  lies between the Wigner and the Husimi function.

For Gaussian superpositions one has

$$\mu_{g_{z_1}+g_{z_2}} = \mu_{g_{z_1}} + \mu_{g_{z_2}} + e^{-|z_1-z_2|^2/8h} c_{1,2} \quad (7)$$

where  $c_{1,2}$  is an oscillatory interference term; see Appendix A. Due to the exponentially small prefactor  $e^{-|z_1-z_2|^2/8h}$  the cross term may be neglected for numerical computations whenever the two centers  $z_1$  and  $z_2$  are sufficiently apart from each other.

## IV. NUMERICAL EXPERIMENTS

### A. Accuracy: Gaussian superposition

In a first set of experiments we implement a Quasi-Monte Carlo discretization of our new method (6) in two dimensions with Halton points; see also [4]. We test the accuracy for a Gaussian superposition  $\psi = g_{z_1} + g_{z_2}$ ,  $z_1 = (-1, 1, 1, 1)$ ,  $z_2 = (0, 1, -1, -\frac{1}{2})$ , with varying values of  $h$  and the following observables:

- torsional potential:  $2 - \cos(\hat{q}_1) - \cos(\hat{q}_2)$
- quartic momentum:  $|\hat{p}|^4$

We compare the outcome with reference values from grid based quadrature and do the same for the Husimi method (4); see Figure 4. Since both observables have non-vanishing derivatives of degree four, the errors of the spectrogram method are of size  $O(h^2)$ . In contrast, for the Husimi method (4), the expectation values are approximated with  $O(h)$  accuracy only.

### B. High dimensions: Henon–Heiles

In a second set of experiments we show the applicability of the new method in moderately high dimensions. We consider the Henon–Heiles Hamiltonian

$$\begin{aligned} \hat{H} &= -\frac{h^2}{2} \Delta + \sum_{j=1}^d \frac{q_j^2}{2} + \alpha \sum_{j=1}^{d-1} (q_j^2 q_{j+1} - \frac{q_{j+1}^3}{3}) \\ &=: \frac{1}{2} |\hat{p}|^2 + V_d(q) \end{aligned} \quad (8)$$

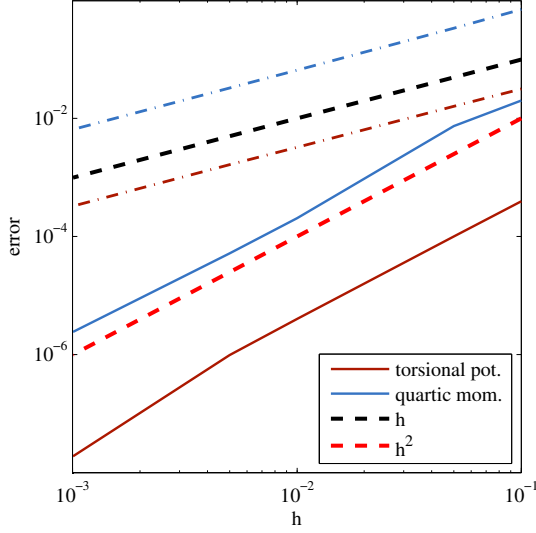


Figure 4. Approximation errors of expectation values for the spectrogram method (6) (solid lines) and the Husimi method (4) (dashed dotted lines).

with  $\alpha = 1.8436$  and  $h = 0.0037$  in dimensions  $d = 2, \dots, 128$ , and a Gaussian state  $\psi = g_z$  centered in  $z = (q, p)$  with  $q_1 = \dots = q_d = 0.3645$  and nonzero momentum  $p_1 = 1, p_2 = \dots = p_d = 0$ .

The Hamiltonian  $\hat{H}$  and the state  $\psi$  constitute a benchmark system for time-dependent propagation methods; see e.g. [12, 13]. Since the potential function  $V_d$  is a polynomial of degree three, the spectrogram method (6) gives the exact kinetic and potential energies, and all errors are sampling errors, see Figure 5.

## V. CONCLUSION

We have suggested a new phase space density for computing quantum expectation values by taking a linear combination of spectrograms. The new phase space density not only remedies the difficulty in sampling with the Wigner function but also provides a higher-order approximation of observables than the Husimi function

in the high frequency regime.

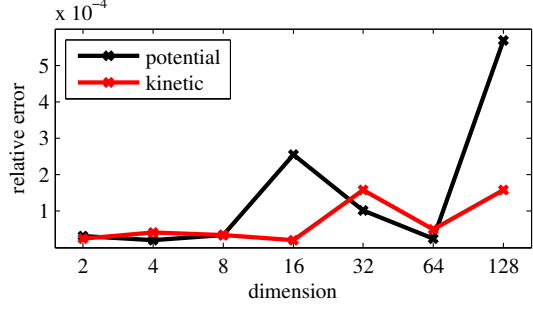


Figure 5. Relative Henon-Heiles energy errors in dimensions  $d = 2, \dots, 128$  with  $10^8$  Monte-Carlo points.

## Appendix A: Cross terms

For the Gaussian superposition  $\psi = g_{z_1} + g_{z_2}$ , both the Wigner function and the new density contain an oscillatory cross term that localizes around the arithmetic mean  $z_+ = \frac{1}{2}(z_1 + z_2)$ . For the Wigner function, we have

$$\mathcal{W}_\psi = \mathcal{W}_{g_{z_1}} + \mathcal{W}_{g_{z_2}} + 2\gamma_{1,2}$$

with

$$\gamma_{1,2}(z) = (\pi h)^{-d} \exp(-\frac{1}{h}|z - z_+|^2) \times \cos(\frac{1}{h}(z_1 - z_2) \cdot \Omega z),$$

where

$$\Omega := \begin{pmatrix} 0 & \text{Id}_{d \times d} \\ -\text{Id}_{d \times d} & 0 \end{pmatrix} \in \mathbb{R}^{2d \times 2d}.$$

For the new density, we obtain equation (7) with cross term

$$\begin{aligned} c_{1,2}(z) &= (2\pi h)^{-d} \exp(-\frac{1}{2h}|z - z_+|^2) \\ &\times \left( (z - z_1) \cdot (z - z_2) \cos(\frac{1}{2h}(z_1 - z_2) \cdot \Omega z) \right. \\ &\quad \left. - (z - z_1) \cdot \Omega(z - z_2) \sin(\frac{1}{2h}(z_1 - z_2) \cdot \Omega z) \right) \end{aligned}$$

In comparison to the Wigner function, the cross term of the new density is damped by the small constant  $e^{-|z_1 - z_2|^2/8h}$ .

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